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Novel Materials

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Introduction

Novel materials with significantly new properties are arising from the ability to create materials with nanoscale structures. Such nanoscale materials often exhibit unique and optimized properties without bulk analogues. Microelectromechanical systems (MEMS), which combine electronics with mechanical devices, offer new levels of technology. New challenges in understanding and predicting the materials properties, design, and processing come with these systems. Needs in computation for predicting the properties and response of micro/nano-scale materials range from fundamental calculations of materials properties to simulations of system behavior. The main areas of interest for research in micro/nano-scale systems are described here.

Nanoscience Based Materials Design and Process

One of the distinguishing features of many nanomaterials is self-assembly of the molecules into a structure. While some understanding of the self-assembly process exists, we need to be able to predict the self-assembled structure from the molecule components and the process conditions. The assembly of multicomponent systems, particularly systems that develop multiple, hierarchical levels of assembly has hardly been studied. In addition to self-assembly into a final, static structure, active self-assembly, in which the self-assembly can be driven by an external input from one state to another, is a main interest. The ability to use self-assembly to control and produce nanoscale patterns in materials is an important characteristic and needs to be studied. The production of well-dispersed nanocomposites is another self-assembly process that is of particular interest.

Another defining characteristic is the new phenomena that occur because interfaces and free surfaces have significant influence at the nanoscale. Integration of nanodevices in microsystems demands that different materials be brought together and that the interfaces between materials not traditionally considered be understood at a fundamental level. For example, the description of the interface between a polymer and a metal is a challenge for present atomistic simulations; force-fields with the necessary predictive power have not been developed for such mixed systems, while quantum electronic structure calculations are unable to handle the relevant length and time scales. Further, techniques that sample the large phase space of these complex interfaces to determine the equilibrium and/or kinetics-driven atomic structure are required. The high surface-to-volume ratio of nanoparticles means the surface properties are important and can, in some instances, dominate the materials' properties and response. Often, the surface properties are fundamentally different from bulk properties.

In order to predict the nanoscale structures, the atomic interactions must be well characterized. Besides the fundamental calculations of bond strength necessary for material strength, there is a general need for quantum chemistry calculations and other first-principles approaches. The effects of nanoscale confinement on chemical reactions and the behavior of defects and impurities need to be calculable. Thus force-fields that are reliable for transition states and equilibrium conditions are required as well as methodologies for the efficient determination of reaction mechanisms and rates in complex systems. As noted above a major weakness is the ability to simulate dissimilar materials over the length and time scales characteristic of nanoscale systems. Calculations of force fields for mixed systems and further development of quantum/classical hybrid techniques are a basic need.

The electrical and optical properties depend on the quantum nature of the material. There is a need for large-scale quantum mechanical calculations of the electrical and optical properties of the materials. In order for these methods to be applicable to large systems, they should scale linearly with the number of electrons and must be able to utilize massively parallel computational resources. The underlying numerical techniques must be sufficiently robust to study systems comprised of highly dissimilar materials.

The treatment of many-body interactions, correlation effects in electrons and photon-matter interactions is important. In addition, first-principles calculations of excited states in materials are important for the accurate predictions of the optical properties. Traditional techniques such as the Local Density Approximation and the Generalized Gradient Approximation that are designed to determine ground state properties frequently produce large errors when applied to electronic excited states. Further development of quantum mechanical capabilities aimed at dynamic electronic properties is needed.

The mechanical strength of a material is an essential property to guide the synthesis of novel micro/nano-scale materials and systems. The nanoscale presents new issues related to the small length scales. Materials may be composed of one or just a few grains, which fundamentally alters their mechanical properties compared to their bulk properties. Predicting the strength and stability of material interfaces is a topic of significant interest. The atomic scale deformation mechanisms and the failure initiation need to be calculable. Materials, such as nanocomposites, which offer high material strength combined with other properties are of particular interest.

Nanodevice / Microsystems Fabrication and Integration

Besides material properties, deposition and fabrication of a material must be modeled with high fidelity. For example, in a fabrication process which consists of multiple steps of deposition, etching and annealing treatments, how each treatment ultimately affects the final material properties is a key issue. In particular, the process-induced residual stress

needs to be predicted.

Thermal transport between the multiple materials that can exist in a microsystem must be calculable, in order to determine the effects of high temperature processing on the system components. In a similar vein, heat transport is important to understand in the integration process. The heat generated by one part of the device can raise the temperature of another part, which may not generate heat on its own, but may not function well in the presence of 'external' heat. This requires the ability to calculate thermal transport across a system with nanoscale parts that span micrometers.

Performance and Reliability Prediction for Microsystems and Nanodevices

The systems are typically composed of many parts. The performance and reliability depends on the individual parts function and the interaction between all the parts. Thus, there is the need to model interaction between the parts in a microsystem. This can include a hierarchical approach of modeling the interactions within a subassembly and the interactions among the subassemblies. Besides interactions within a device, the aging, safety and reliability of devices in various end-use and service environments must be predicted. Ultimately, the ability to predict damage and failure due to any source is needed.

The moving parts of mechanical devices make stiction, friction and wear key phenomena that need to be better understood and predicted. Modeling and simulation should help design the coating material and model the coating process. The necessary conditions to yield good coverage need to be understood. The effect of the environment (e.g. humidity) on the reliability of coating needs to be predicted.

Fluctuations and microscopic variability play an increasingly important role in device performance as device sizes are scaled down. Smaller components inherently have fewer degrees of freedom and so noise and fluctuations become a larger fraction of the relevant properties. Variability of properties is also more significant at smaller scales. These fluctuations and variability must be incorporated in to the overall device modeling in order to determine reliability and the range of device performance. Methodologies for determining these variations and convoluting them into overall device performance need to be developed.

Novel Methodology Development

In order to meet the challenges for the above problems, novel theoretical and simulation methodologies need to be developed. Major challenges exist for simulating micro/nano-scale systems over a realistic range of time, length, temperature, etc. as well as multiple physical conditions and environments.

Validation and Verification (V&V)

For all the above interests, validation and verification are also required. Verification is the
process of determining that a computer simulation correctly represents the conceptual model and its solution – i.e., that the simulation approach has solved the problem correctly. Validation is the process of determining the degree to which a computer simulation is an accurate representation of the real world – i.e., that the simulation approach has solved the correct problem. Synchronization of code validation and experimental programs is a high priority of the V&V program. The needed experimental data required to assess code fidelity will be supported.

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